Geophysical Research Abstracts, Vol. 7, 11066, 2005 SRef-ID: 1607-7962/gra/EGU05-A-11066 © European Geosciences Union 2005



Three-Dimensional Chemical Analysis with Synchrotron X-ray Tomography and Prospects with Neutron Tomography

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Synchrotron X-ray tomography was used to image, at 3.34 micron resolution, a mixture containing high-impact polystyrene (HIPS) and a two-component flame retardant, a brominated phthalimide dimer (SaytexTM BT-93) and a synergist, antimony oxide (Sb₂O₃). The two components are nicely compatible with X-ray tomography. Complete tomography data sets were acquired at seven X-ray energies in the range of 12 to 40 keV, closely spanning Br and Sb 1s electron binding energies at 13.474 and 30.491 keV, respectively. The images were converted to 3D chemical concentration distribution [Ham, 2004]; the images show a spatial correlation between the two components that is attributed to the mixing order.

What is the future of "chemical analysis"? In the 1800's, it meant dissolving a sample in strong acid. In the 1900's, it meant injection into a "spectrometer" and line spectra interpretable by a few experts. Now, chemical analysis can mean three-dimensional imaging with methods such as X-ray tomography, MRI, neutron tomography, or electron microscope tomography. This research will exploit these imaging methods to develop high throughput chemical analysis procedures. The initial work has been followed with more X-ray tomography on even more complex polymer blends. The flame retardant industry is also producing non-bromine additives such as phosphonates. These are not compatible with X-ray tomography, hence our interest in neutron tomography. One question is how munc of the X-ray tomography analysis can be transferred to the neutron images.

Three-Dimensional Chemical Analysis: Synchrotron Tomography at Multiple X-ray Energies of Brominated Aromatic and Antimony Oxide Additives in Polystyrene." Ham, K.; Jin, H.; Al-Raoush, R.; Xie, X.; Willson, C. S.; Byerly, G. R.; Simeral, L. S.; Rivers, M. L.; Kurtz, R. L.; Butler, L. G. Chemistry of Materials, **2004**, 16, 4032-42.